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Effects of unsaturated fatty acids (Arachidonic/Oleic Acids) on stability and structural properties of Calprotectin using molecular docking and molecular dynamics simulation approach

Nematollah Gheibi[1], Mohamad Ghorbani[2], Hanifeh Shariatifar[3], Alireza Farasat[1]*

1 Cellular and Molecular Research Center, Research Institute for Prevention of Non Communicable Diseases, Qazvin University of Medical Sciences, Qazvin, Iran, **2** Department of Nanobiotechnology/ Biophysics, Faculty of Biological Science, Tarbiat Modares University, Tehran, Iran, **3** Young Researchers and Elite Club, Tehran Medical Sciences, Islamic Azad University, Tehran, Iran

* a.farasat@qums.ac.ir

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Abstract

Calprotectin is a heterodimeric protein complex with two subunits called S100A8/A9. The protein has an essential role in inflammation process and various human diseases. It has the ability to bind to unsaturated fatty acids including Arachidonic acid, Oleic acid and etc., which could be considered as a major carrier for fatty acids. In this study we aimed to appraise the thermodynamics and structural changes of Calprotectin in presence of Arachidonic acid/Oleic acid) using docking and molecular dynami simulation method. To create the best conformation of Calprotectin-Oleic acid/Arachidonic acid complexes, the docking process was performed. The complexes with the best binding energy were selected as the models for molecular dynamics simulation process. Furthermore, the structural and thermodynamics properties of the complexes were evaluated too. The Root Mean Square Deviation and Root Mean Square Fluctuation results showed that the binding of Arachidonic acid/ Oleic acid to Calprotectin can cause the protein structural changes which was confirmed by Define Secondary Structure of Proteins results. Accordingly, the binding free energy results verified that binding of Oleic acid to Calprotectin leads to instability of S100A8/A9 subunits in the protein. Moreover, the electrostatic energy contribution of the complexes (Calprotectin-Oleic acid/Arachidonic acid) was remarkably higher than van der Waals energy. Thus, the outcome of this study confirm that Oleic acid has a stronger interaction with Calprotectin in comparison with Arachidonic acid. Our findings indicated that binding of unsaturated fatty acids to Calprotectin leads to structural changes of the S100A8/A9 subunits which could be beneficial to play a biological role in inflammation process.

1. Introduction

The S100A8/A9 or Myeloid Related Proteins (MRP8/ MRP14) are two small proteins which structurally belong to S100 protein family [1, 2]. The S100A8/A9 protein complex